

(FILE 'HOME' ENTERED AT 14:32:10 ON 29 JUL 2003)

FILE 'REGISTRY' ENTERED AT 14:32:24 ON 29 JUL 2003

E DECYLISONONYLDIMETHYLAMMONIUM CHLORIDE/CN
E DECYL ISONONYLDIMETHYLAMMONIUM CHLORIDE/CN
E ISONONYLDECYLDIMETHYLAMMONIUM CHLORIDE/CN
E ISONONYL DECYLDIMETHYLAMMONIUM CHLORIDE/CN
E DIMETHYLDECYLISONONYLAMMONIUM CHLORIDE/CN

FILE 'CAPLUS, BIOSIS, MEDLINE' ENTERED AT 14:34:57 ON 29 JUL 2003

L1 6 S DECYLISONONYLDIMETHYLAMMONIUM
L2 5 S N-DECYL-N-ISONONYL-N,N-DIMETHYLAMMONIUM
L3 2 S L2 NOT L1

FILE 'REGISTRY' ENTERED AT 14:55:50 ON 29 JUL 2003

E DIDAC/CN

L5 ANSWER 17 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1951:29541 CAPLUS

DN 45:29541

OREF 45:5100c-e

TI **Invert soaps** as disinfectants. III

AU Tanaka, Fukuju; Inouye, Itaru; Namba, Yataro

CS Takeda Pharm. Inds., Ltd., Tokyo

SO Yakugaku Zasshi (1943), 63, 353-64

CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Unavailable

CC 10 (Organic Chemistry)

AB The following compds. were synthesized and their germicidal power tested: Dodecyldimethylphenylammonium Me sulfate and compds. in which the Ph radical has been changed to p-, .omicron.-, and m-MeOC₆H₄, .omicron.-, and p-tolyl, and p-phenctyl radicals; **dodecyl**(p-methoxyphenyl)dimethylammonium chloride; methylethyldodecylphenylammonium Et sulfate; (p-dodecylphenyl)trimethylammonium Me sulfate; dimethylcetylphenylammonium Me sulfate and compds. in which the Ph radical has been changed to p-MeOC₆H₄ and p-tolyl radicals; 1-dodecylpyridinium chloride as one of pyridinium salts, and compds. in which its 1-**dodecyl** radical has been changed to hexadecylcetyl, (carbododecyloxymethyl) and 1-(2-lauroyloxyethyl); 1-carbododecyloxymethylpicolinium chloride; dimethylbenzyl(2-lauroyloxyethyl)ammonium chloride; diethylbenzyl(2-lauroyloxyethyl)ammonium chloride. Germicidal action against B. coli was found to be greatest in (dodecyloxyethyl)pyridinium chloride, being 1.75 times as strong as Zephirol.

IT Disinfectants and Antiseptics

(of alkylbenzyldimethylammonium chlorides, chem. constitution and action of)

IT Ammonium, (2-ethoxyethyl)hexadecyldimethyl-, chloride
Ammonium, (p-dodecylphenyl)trimethyl-, methyl sulfate
Ammonium, benzyl(2-hydroxyethyl)dimethyl-, chloride, laurate
Ammonium, benzyldiethyl(2-hydroxyethyl)-, chloride, laurate
Ammonium, **dodecyl**(p-ethoxyphenyl)dimethyl-, methyl sulfate
Ammonium, **dodecyl**(p-methoxyphenyl)dimethyl-, chloride
Ammonium, **dodecyl**[m-methoxyphenyl]dimethyl-, methyl sulfate
Ammonium, **dodecyl**[o-methoxyphenyl]dimethyl-, methyl sulfate
Ammonium, **dodecyl**[p-methoxyphenyl]dimethyl-, methyl sulfate
Ammonium, dodecyldimethyl-o-tolyl-, methyl sulfates
Ammonium, dodecyldimethyl-p-tolyl-, methyl sulfates
Ammonium, dodecyldimethylphenyl-, methyl sulfate
Ammonium, dodecylethylmethylphenyl-, ethyl sulfate
Ammonium, hexadecyl(2-methoxyethyl)dimethyl-, chloride
Ammonium, hexadecyl(p-methoxyphenyl)-dimethyl-, methyl sulfate
Ammonium, hexadecyldimethyl-p-tolyl-, methyl sulfate
Ammonium, hexadecyldimethylphenyl-, methyl sulfate
Picolinium compounds, 1-(carboxymethyl)--, chloride, **dodecyl** ester
Pyridinium, 1-(2-hydroxyethyl)-, chloride, laurate
Pyridinium, 1-(carboxymethyl)-, chloride, **dodecyl** ester
IT 104-74-5, Pyridinium, 1-**dodecyl**-, chloride 123-03-5,
Pyridinium, 1-hexadecyl-, chloride 959-55-7, Ammonium,
benzyldimethyloctyl-, chloride 17177-93-4, Ammonium,
hexadecyldimethyl(2-phenoxyethyl)-, chloride
(prepn. of)

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AN 1951:29540 CAPLUS

DN 45:29540

OREF 45:5099i,5100a-c

TI **Invert soaps** as disinfectants. II

AU Tanaka, Fukuju

CS Takeda Pharm. Inds., Ltd., Tokyo

SO Yakugaku Zasshi (1943), 63, 343-53

CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Unavailable

CC 10 (Organic Chemistry)

AB cf. C.A. 44, 11037i. To obtain quaternary ammonium salts with powerful germicidal properties, T. synthesized the following new compds. of which those marked with asterisks (*) showed especially powerful action against Escherichia coli: (1) Ketones: Dodecylpiperidinium chlorides: phenacyl, p-chlorophenacyl, and acetonyl. Dodecyldimethylammonium chlorides: phenacyl, p-chlorophenacyl*, acetonyl*, 2,5-dichlorophenacyl*, and p-methoxyphenacyl*. Dodecyldiethylammonium chlorides: phenacyl, p-chlorophenacyl, 2-methyl-3-oxobutyl, 2-ethyl-3-oxopropyl, 2-ethyl-3-oxoamyl, and acetonyl. Acetonylhexadecyldimethylammonium chloride was also prepd. (2) Amides: Me2(C12H25)RNCl, R given: AcNH, AcPhN*, Ac(p-ClC6H4)N, Ac(2,5-Cl2C6H3)N, Ac(.omicron.-MeC6H4)N, AcEtN, Ac(p-MeOC6H4)N, Ac(p-EtOC6H4)N, and Ac(p-MeC6H4)N*. Et2(C12H25)(AcNH)NCl, Me2(C16H33)(AcNH)NCl, and Me2(C16H33)(AcPhN)NCl were also prepd. (3) Ethers: Me2(C12H25)RNCl, R given: MeO(CH2)2, Me2CHCH2O(CH2)2*, Me2CH(CH2)2O(CH2)2*, PhO(CH2)2*, PhCH2O(CH2)2*, .omicron.-ClC6H4CH2O(CH2)2*, p-BrC6H4CH2O(CH2)2*, and PhOCH2CH(OH)CH2. Me2(C16H33)RNCl were prepd. (R given): MeO(CH2)2, EtO(CH2)2, PhO(CH2)2, PhCH2O(CH2)2.

IT Disinfectants and Antiseptics

(ammonium compds. (quaternary))

IT Surface-active substances (capillary- or interface-active substances)

(ammonium compds. (quaternary), as disinfectants)

IT Ammonium, (1-carbamoylpropyl)dodecyldimethyl-, chloride
Ammonium, (2,5-dichlorophenacyl)dodecyldimethyl-, chloride
Ammonium, (2-ethoxyethyl)hexadecyldimethyl-, chloride
Ammonium, (carbamoylmethyl)dodecyldiethyl-, chloride
Ammonium, (.alpha.-carbamoyl-2,5-dichlorobenzyl)dodecyldimethyl-, chloride
Ammonium, (.alpha.-carbamoyl-p-chlorobenzyl)dodecyldimethyl-, chloride
Ammonium, (.alpha.-carbamoyl-p-ethoxybenzyl)dodecyldimethyl-, chloride
Ammonium, (.alpha.-carbamoyl-p-methoxybenzyl)dodecyldimethyl-, chloride
Ammonium, (.alpha.-carbamoylbenzyl)dodecyldimethyl-, chloride
Ammonium, (.alpha.-carbamoylbenzyl)hexadecyldimethyl-, ammonium chloride
Ammonium, (p-chlorophenacyl)dodecyldiethyl-, chloride
Ammonium, (p-chlorophenacyl)dodecyldimethyl-, chloride
Ammonium, [(2-(o-chlorobenzoyloxy)ethyl)dodecyldimethyl-, chloride
Ammonium, [2-(benzyloxy)ethyl)dodecyldimethyl-, chloride
Ammonium, [2-(benzyloxy)ethyl]hexadecyldimethyl-, chloride
Ammonium, [2-(p-bromobenzoyloxy)ethyl)dodecyldimethyl-, chloride
Ammonium, acetonyldodecyldiethyl-, chloride
Ammonium, acetonyldodecyldimethyl-, chloride
Ammonium, acetonylhexadecyldimethyl-, chloride
Ammonium, **dodecyl**(2-isobutoxyethyl)dimethyl-, chloride
Ammonium, **dodecyl**(2-methoxyethyl)dimethyl-, chloride
Ammonium, **dodecyl**(p-methoxyphenacyl)dimethyl-, chloride
Ammonium, **dodecyl**[2-(isopentoxo)ethyl]dimethyl-, chloride
Ammonium, dodecyldiethyl(2-ethyl-3-oxopentyl)-, chloride
Ammonium, dodecyldiethyl(2-formylbutyl)-, chloride
Ammonium, dodecyldiethyl(2-methyl-3-oxobutyl)-, chloride
Ammonium, dodecyldiethylphenacyl-, chloride
Ammonium, dodecyldimethylphenacyl-, chloride

Ammonium, dodecyldimethylphenyl-, methyl sulfate
 Ammonium, dodecylethylmethylphenyl-, ethyl sulfate
 Ammonium, hexadecyl(2-methoxyethyl)dimethyl-, chloride
 Piperidinium compounds, 1-(p-chlorophenacyl)-1-**dodecyl**-,
 chloride
 Piperidinium compounds, 1-acetonyl-1-**dodecyl**-, chloride
 Piperidinium compounds, 1-**dodecyl**-1-phenacyl-, chloride
 IT Ammonium, [.alpha.-carbamoyl-o-methylbenzyl]dodecyldimethyl-
 Ammonium, [.alpha.-carbamoyl-p-methylbenzyl]dodecyldimethyl-
 (chlorides)
 IT 14798-03-9, Ammonium
 (compds., substituted, as disinfectants)
 IT 4728-59-0, Ammonium, **dodecyl**(2-hydroxy-3-phenoxypropyl)dimethyl-
 , chloride 10561-60-1, Ammonium, dodecyldimethyl(2-phenoxyethyl)-,
 chloride 15538-15-5, Ammonium, (carbamoylmethyl)dodecyldimethyl-,
 chloride 15646-40-9, Ammonium, (carbamoylmethyl)hexadecyldimethyl-,
 chloride 17177-93-4, Ammonium, hexadecyldimethyl(2-phenoxyethyl)-,
 chloride 17697-46-0, Piperidine, 1-(2-methyl-2-nitropropyl)-
 (prepn. of)

L5 ANSWER 29 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

TI **Invert soaps.** VI. Triazolium salts

AB Monoalkyltriazaoles, probably the 1-isomers, are obtained in 60-80% yield by the action of alkyl chlorides on K benzotriazole; the mother liquors contain the 2-isomers. Using alkyl bromides the 1,3-dialkylbenzotriazolium bromides result. The 1,3-diethyl-, -dibutyl- and -dibenzylbenzotriazolium bromides have practically no action on lactic-acid bacteria; the effects of octyl, **dodecyl** and cetyl groups are approximately as 4:2:1. The most effective disinfectants against pernicious bacteria are those with 2 different alkyls, e. g., 1-**dodecyl**-3-ethylbenzotriazolium bromide. For comparison with the benzotriazolium salts, some 1,2,4-triazole derivs. were also prepd. The solid K salt of 1,2,4-triazole was prepd. by treatment of 7.5 g. 1,2,4-triazole with KOEt and addn. of ether; yield, 10.9 g. of white crystals. On heating with 22 g. **dodecyl** chloride and 16 cc. EtOH for 16 hrs. at 110.degree., N-dodecyltriazole (I), C14H27N3, was obtained as rhombic plates with pearly luster, m. 39.degree., sol. in org. solvents and dil. acids, insol. in H2O. When I is heated with 1.1 moles EtBr at 100.degree. for 14 hrs., N-**dodecyl**-1,2,4-triazole-EtBr (II) C16H32N3Br, is obtained quantitatively as large leaves from 5:1 AcOEt-alc., m. 150-2.degree.. N-Dodecylbenzotriazole (III), C18H29N3, was prepd. from 8 g. K benzotriazole and 10.4 g. **dodecyl** chloride in 10 cc. alc.; yield, 10.5 g. crystals from petr. ether, m. 44-6.degree.; methosulfate, C20H35O4N3S, large leaves, m. 25.degree.; ethobromide, C20H34N3Br, m. 27.degree.; butobromide, C22H38N3Br, rosette leaves from EtOAc-petr. ether, m. 33.degree.. N-Cetylbenzotriazole (IV), C22H37N3, prepd. as was III, flat rectangular platelets from alc., m. 62.degree. (yield 70%); methosulfate, C24H44N3O4S, rhombohedrons, m. 76-7.degree.; ethobromide, lancet-shaped leaves in stars, m. 96-7.degree.. 1,3-Dioctylbenzotriazolium bromide (V), C22H38N3Br, was prepd. from K benzotriazole and 2 moles octyl bromide, shining leaflets from EtOAc, m. 147-8.degree.. 1,3-Didodecylbenzotriazolium bromide, C30H54N3Br, intertwined silky needles from EtOAc, m. 141-3.degree.. 1,3-Dibenzylbenzotriazolium chloride, C20H18N3Cl, prepd. using 2 moles PhCH2Cl, cubes from EtOH-AcOEt, m. 207-9.degree., has a bitter taste.

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